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A1

Graph Automorphism Perception Algorithms in Computer-Enhanced Structure Elucidation

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The concept of graph symmetry is explained in terms of the vertex automorphism group, which is a subgroup of the complete vertex permutation group. The automorphism group can be deduced from the automorphism partition of graph vertices. An algorithm is described which constructs the automorphism group of a graph from the automorphism vertex partitioning. The algorithm is useful especially for graphs which contain more than one vertex-partition set. Several well-known topological symmetry perception algorithms that yield automorphism partitions are compared. The comparison is favorable to the Shelley–Munk algorithm, developed in the framework of the SESAMI system for computer-enhanced structure elucidation.

INTRODUCTION

Most computer programs that require the manipulation of chemical structures among their operations (e.g., computer-enhanced structure elucidation, spectrum interpretation and simulation, and synthetic design) must eventually be able to recognize and process stereochemical information if they are to be truly useful.[1] There are different approaches to the treatment of stereochemistry[2] and related problems, but all of them share in common the need to consider the symmetry of the molecular structure under consideration.

Symmetry properties of molecular structures are very important because they are reflected in a variety of molecular properties, interactions, and other structure-related phenomena.[3] For the correct interpretation of some experimentally derived information, e.g., X-ray diffraction patterns or IR spectra, the determination of molecular stereogeometry is necessary; this implies the use of group theory formalism in the determination of appropriate space or point groups and their elements. In some other areas, like computer-enhanced structure elucidation[4] or the enumeration of ^{13}C-NMR signals,[5] partial solutions are possible using topological symmetry (connectivity) instead of three-dimensional geometry. For such cases, a different concept of symmetry, based on graph theory, can be used to advantage.[6]

The objective of this article is to describe the connection between the automorphism partitioning of the vertices of graphs and the automorphism groups of graphs. An algorithm to construct the automorphism group from the automorphism partition of the vertices is presented. Several procedures to obtain the automorphism partitioning of graphs, including graphs containing isospectral points, are compared with the Shelley–Munk algorithm.[7,8] A critical comparison shows, contrary to the perception in the literature,[9,10] that the algorithm is rigorous and efficient and distinguishes isospectral points without difficulty.

SYMMETRY OF GRAPHS

The properties of a graph do not depend on its pictorial representation, but only on its connectivity. Thus, a graph, which can be drawn in several different ways, may appear to possess different symmetry elements in the normal sense of point group symmetry; however, the topological symmetry of each representation is identical based on connectivity. This aspect makes the consideration of graph symmetry quite different from the conventional molecular point group and space group approaches. (This is discussed with examples in ref 11.)

In terms of graph theory, the structural symmetry relates to the vertex automorphism group: this group is a subgroup of the complete vertex permutation group of the graph representing the chemical structure.[12,13] Mathematically, these relations can be expressed simply and succinctly by using matrix algebra. The two matrices used in the following relations are the adjacency matrix A and the permutation matrix P defined as

$$A_{ij} = \begin{cases} 1 \text{ if vertices } i \text{ and } j \text{ are neighbors} \\ 0 \text{ otherwise} \end{cases}$$

$$P_{ij} = \begin{cases} 1 \text{ if a mapping of vertices } i \longrightarrow j \text{ is induced by the given permutation of vertices} \\ 0 \text{ otherwise} \end{cases}$$

There are $n!$ possible labelings of a graph with n vertices. Each of them can be represented by a vector $\mathbf{P}$, and the transformation between two different labelings is given by the permutation matrix P.

In Figure 1, three of 120 possible labelings of a graph are shown together with the corresponding adjacency matrices A and permutation vectors $\mathbf{P}$. Although the graphs G_1 and G_2 represent the same structure, they are not identical because of the different labelings of their vertices, i.e., different connectivity. Since they represent the same structure, they are known as isomorphic graphs. The isomorphism can be expressed mathematically with the following relations, holding generally for all graphs:

$$P_{12}^{1} \cdot A(G_1) \cdot P_{12} = A(G_2) \tag{1}$$

Because the permutation matrix is an orthogonal matrix, its inverse is equal to its transpose, and the relation can be further simplified:

$$P_{12}^{T} \cdot A(G_1) \cdot P_{12} = A(G_2) \tag{2}$$

Such a transformation is called an isomorphism between the graphs G_1 and G_2. Figure 2 shows the matrices and the results of matrix multiplication for the expression 2: the permutation matrix P_{12} expresses the mapping $P_1 \cdots P_2$ and the consecutive multiplication of $A(G_1)$ with P_{12} and P_{12}^{T} results in $A(G_2)$.

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‡ Camille and Henry Dreyfus Teacher-Scholar.

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